

Benzene

71-43-2 | DTXSID3039242

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 50.5 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.58e-01

Confidence level: 6.77e-01

Nearest Neighbors from the Training Set

Image not found

Benzene

Measured: 56.2

Predicted: 50.5

Image not found

Phenol

Measured: 26.9

Predicted: 57.3

Image not found

Toluene

Measured: 117

Predicted: 87.4

Image not found

Resorcinol

Measured: 9.55

Predicted: 28.3

Image not found

Chlorobenzene

Measured: 141

Predicted: 106